ABSTRACT

Computer-based methods for modeling complex formation between a query ligand and a target macromolecule are described herein. The methods can include, for example, providing a structural model of a query ligand and a structural model of a target macromolecule; identifying a substructure of the query ligand; identifying comparison ligands in a set of 3-D structural models that each share an identical substructure with the query ligand, wherein each 3-D structural model comprises a comparison ligand and a comparison macromolecule, and wherein the comparison macromolecule has structural features homologous to the target macromolecule; mapping spatial relationships between the substructure atoms of the query ligand and the comparison ligand such that corresponding atoms are identified; assigning atomic coordinates to the corresponding atoms of the query ligand; and generating one or more output models, each model comprising a 3-D structural model of the query ligand substructure and the target macromolecule. Related articles and apparatuses are also described.